

Magnetic destabilization of Ni₇Al

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Previously unknown cubic ordered Ni₇Al and Cu₇Pt compounds have recently been theoretically predicted to be stable phases in the Ni-Al and Cu-Pt systems. While Cu₇Pt was subsequently synthesized and identified,

to an Ising-like model, which was then used to predict the energies of other phases not calculated (such as $D7$). ^{~ii!} The previous approach for Ni-Al (but not Cu-Pt! -Ref. 3! utilized LDA energies based on the method of linear muffin-tin orbitals within the atomic sphere approximation (LMTO-ASA) rather than a full-potential approach. ^{~iii!} Nonmagnetic calculations were employed. Due to the absence of experimen-

values of exchange splitting and bandwidth.¹⁸⁻²¹ The calculated magnetic moment in pure Ni ($0.59 m_B/\text{atom}$) is in good agreement with the observed value ($0.61 m_B/\text{atom}$); however, as in previous calculations,²²⁻²⁵ the calculated magnetic moment of Ni in the Ni₃Al compound ($0.20 m_B/\text{atom}$) is higher than the experimental value ($0.08 m_B/\text{atom}$).²⁶

~3! Implication of Magnetism on Superlattice Stability:
The destabilization of the Ni₇Al structure with spin polarization also has interesting consequences on the calculated Ni/Ni₃Al interfacial energies. The energy of a coherent A_pB_p superlattice between materials A and B can be separated into two components:²⁷ ~a! *Coherency Strain*: the strain energy required to maintain coherency between the ~lattice mismatched! materials A and B, and ~b! *Interfacial Energy*: the energy associated with the interactions between materials at the A/B interface-s!. To define these terms, it is useful to first

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¹T. B. Massalski, *Binary Alloy Phase Diagrams* ~ASM International, Metals Park, OH, 1986!

²R. Hultgren, R. D. Desai, D. T. Hawkins, M. Gleiser, and K. K. Kelley, *Selected Values of the Thermodynamic Properties of Binary Alloys* ~